

1P24

Theoretical study on Sextuple Bond in Dinuclear Transition Metal Complex

○陳 躍¹, 榊 茂好², 長谷川 淳也¹

¹北大触媒研, ²京大福井センター

chenyue@cat.hokudai.ac.jp

At present, most studies of sextuple bond are focused on the diatomic molecules, but the complex with metal-metal sextuple bond has not been reported yet. In this work, we will theoretically present a scheme to achieve the transition metal-metal sextuple bond in dinuclear complexes, where the electron donating and neutral tetradentate ligand is employed, like 12-crown-4 ether (referred as O₄). In diatomic molecules, the sextuple bond exists stably in W₂ and Mo₂, but it can not be formed stably in Re₂²⁺ and Tc₂²⁺. While M₂ (M = W, Mo, Re⁺, Tc⁺) coordinated with two O₄ ligands forming end-on coordinating complex O₄(M₂)O₄, the sextuple bond are achieved in W, Mo, and Re complexes with effective bond order of 5.17, 5.10, and 4.76, respectively. The achievement of sextuple bond is because (1) tetradentate electron donating ligand coordination will destabilize both (n+1)s and nd orbitals to keep the orbital orders relatively unchanged (2) the charge neutrality could prevent from the strong coordination that will destabilize the (n+1)s orbital much more. On the other hand, the charge transfer from ligand metal centers can stabilize the total system. Actually, all these complexes exhibit large formation energy, indicating the possibility of synthesis.